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Astrophysical Simulations as Virtual Labs

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An exploding supernova is not an experiment for the laboratory. Nor is a phenomenon at another extreme of time scales: the slow motion and evolution of galaxies—observers would be skeletal remains long before they could see anything interesting. Extreme ranges of energy and time scales, and the very inaccessibility of the early universe itself, make experimentation impossible and simulation compelling. Astronomers understood this early and did simulations long before they had digital computers. The gears of giant orreries, for example, inspired many formal developments in continued fractions. In 1940, Holmberg built an analog computer to follow the evolution of galaxies. Because light intensity and gravitational forces both decrease like $1/r^2$, a light table became his computer for gravity [4].

Planetoids to the Cosmos

Simulations can help us understand exotic elements and phenomena. Recent decades of precision cosmology have revealed amazing details of the Copernican revolution. We've long known that we aren't at the center of our solar system and live in an unremarkable suburban neighborhood of both our galaxy and the local Virgo cluster of galaxies. Perhaps even more humbling, we now know that most matter isn't in planets and stars. What we are made of is not even the dominant stuff of the universe (dark matter holds that honor), and most of its energy density is some mysterious dark energy that isn't even "stuff" at all. These revelations already glimmered in the 1930s, when astronomers computed that the motions of galaxies within clusters were too fast to be bound by just what was seen. It took four decades for *dark matter* to become fully accepted. Recent observations about dark energy continue to diminish our feelings of self-importance.

Here is the basic argument for the existence of dark energy. We start with Einstein's equations [8]:

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R^{\rho}_{\rho} = 8\pi G\, T_{\mu\nu},$$

where $R_{\mu\nu}$ is the Ricci tensor, R^{ρ}_{ρ} is the curvature scalar, and $T_{\mu\nu}$ is the energy-momentum tensor. A Robertson–Walker metric, $g_{\mu\nu}$, has its space-only metric $g_{ij} = R^2(t)\tilde{g}_{ij}$ scaled by the square of an expansion factor $R(t)$. For an isotropic *gas* and corresponding Robertson–Walker metric, one gets two equations from the t–t and the space–space components of Einstein's field equations, respectively. These are called Friedman's equations (1922):

$$\ddot{R} = 4\pi G\left(\frac{\rho}{3} + p\right)R$$

$$\left(\dot{R}\right)^2 + k = \frac{8\rho G}{3}\rho R.$$

In cosmological simulations, space coordinates are scaled by $R(t)$, $\mathbf{x}(t) = R(t)\mathbf{X}(t)$, and $\mathbf{X}(t)$ are called co-moving coordinates. These $\mathbf{X}$ coordinates are treated in an almost classical fashion because their evolution is slow compared with light speed. In the second of the Friedman equations, $k = K/|K|$, or zero, corresponding to the Gaussian curvature $K = -R^{\rho}_{\rho}/2$. The quantities ρ and p are the energy density and pressure of the gas. If matter dominates, $p = 0$ and $\rho \propto 1/R^3$: $k = -1$ gives $R(t) \propto t$ for large t; for $k = 0$, $R(t) \propto t^{2/3}$, and $k = +1$ makes $R(t)$ a cycloid. In each case, for t in the current epoch, $R(t)$ turns down.

Observationally, it would be hard to decide which k is correct. Recent observations of *standard candles* (Type 1-a supernovae) at high redshift actually show $R(t)$ turning up. Because these supernovae can also be studied locally, we know about their intrinsic brightness. We compare their measured brightnesses, and hence distances, with distances measured by redshift ($R = R_0/(1 + z)$). From these data, $G_{\mu\nu} \to G_{\mu\nu} - \lambda\, g_{\mu\nu}$, i.e., Einstein's "mistake," begins to make sense. His reasoning derived from a stationary universe: From the first Friedman equation shown above, if R = constant, $p = -\rho/3$, and from the second, $\rho = 3k/8\pi GR$. Thus, if $k = +1$, then $p < 0$, but if $k = -1$, $\rho < 0$. As an (unhappy) result, if $R(t)$ = constant, either the energy density is negative or the pressure is negative. With the addition of a $-\lambda g_{\mu\nu}$ term to $G_{\mu\nu}$, we get an *effective pressure*, $p \to p - \lambda/8\pi G$, and an *effective energy density*, $\rho \to \rho + \lambda/8\pi G$. Now, for $k = +1$ or $k = 0$, at large t, $R(t)$ grows exponentially, as in de Sitter or Friedman–Lemaître universes. This is what the standard-candle observations seem to show [10]. The cosmological constant λ represents a form of unobservable energy.

Confirmation of the ubiquitousness of dark energy also comes from nuclear synthesis: Abundances of light versus heavy elements are not consistent with the thermodynamics and acoustical fluctuations for the decoupling of radiation and matter in the early universe (large z). From these and other methods, we can compute that *stuff* or "baryonic matter" is just 4% of the universe, *cold dark matter* is 23%, and some more mysterious *dark energy* is 73%. Most of the baryons are in diffuse plasma. The estimate for the baryonic fraction is also consistent with mass-to-light ratios and counts of galaxies. Vain creatures that we are, we keep gawking at stars, but then they are most of what we can observe and they told us about the dark matter and energy that we have detected only indirectly.

Body Counts

By the late 1950s, light detectors and simulations of astronomical phenomena were incorporating the technology of the digital revolution. Sophisticated numerical integrators were developed [1], but the $O(N^2)$ operation counts restricted the resolution of solar and (harder) large-scale systems. The force on one of N objects is the sum of the contributions from the $N - 1$ others. By symmetry, $N(N - 1)/2$ such forces must be computed at every timestep. For $N \sim 10^8$ or larger, this is a formidable computation. Fortunately, it is not entirely necessary. Two major schemes have been developed for reducing this load. Both rely on the ideas of near- and far-field scale separation.

P^3M Codes. The FFT, the "opposable thumb" of algorithms, was used very early in *Particle–Mesh*, or PM, codes to reduce the convolution of a density function with the Green's function into simple multiplication in Fourier space. With typical cell sizes ranging from 1/3 to 1 times the mean interparticle separation, the code scales as $O(N \log N)$. Cosmological distributions evolve to look highly clustered, even fractal, so information quickly cascades inside a single mesh cell. This can be fixed; the cost is that of fixing the force calculations with a *Particle–Particle* sum on small scales (the combination of PM and P–P is P^3M). The added cost scales as $O(N_k^2)$, where N_k is the number in a local cluster. This can dominate the computation, leading one simulator to lament: "It's a great way to follow clustering until it happens."

Such schemes can become more efficient by making only local adaptations in higher-density regions [2]. Gravity always being attractive, however, clustering develops after long times into very dense regions. Because the dynamical times scale as $(\text{density})^{-1/2}$, adaptive timestepping is required for greater efficiency.

Tree Codes. An alternative multiscale method groups particles into a tree, and particles (or leaves) then ask: "Are you sufficiently far away and compact that I can calculate your force *en masse*?" If the answer is no, child processes are opened and asked the same question. This can be implemented with a simple *opening angle* criterion (the ratio of the tide to the monopole is proportional to the opening angle) or with more complicated error criteria. In the parallel code k_d-grav, expansions are made to hexadecapole order [5] to improve the approximation and give a better ratio of work done to memory fetched. This method retains good scaling properties even with strong clustering and can also work well on solar system simulations.

Hardware versus Algorithms. Microproc-essors have advanced spectacularly since 1965, when Gordon Moore came up with his famous rule. Until very recently, hardware performance doubled about every two years. Algorithm development has largely kept pace, as shown in Figure 1 for N-body simulations. A furious increase in numbers of CPUs in parallel computers since 2000 has made the situation less clear today. Because N-body simulations are not linear systems, the hardware line in Figure 1, for performance in solving $A\mathbf{x} = \mathbf{b}$, tells only part of the story.

What Physics Do We Learn?

Roughly 15 years ago, simulation results became reliable enough to explain newly observed astrophysical phenomena, and sometimes even to make predictions [9]. Galaxy simulations, for example, can say a lot about the production of ellipticals from merging spirals, as well as the production of spheroidal galaxies from fast flyby collisions and tidal beating in clusters (known as "harassment") [7].

Likewise, curiosity about expected cusp forms in cold dark matter (CDM) halos of early dwarf galaxies can be partially satisfied. CDM models usually predict a sharp cusp in density near the center, while observations [6] show flat densities (Figure 2). By coupling N-body simulations with smooth particle hydrodynamics (SPH), it is possible to assess the heating of dark matter from potential fluctuations in bulk matter. Bulk gas motion can be driven by stellar winds and supernovae; gravitational resonances also contribute to bulk gas motions, which heat the dark matter. With the right evolutionary parameters, the CDM becomes warm (WDM), and the core density profiles flatten as observed.

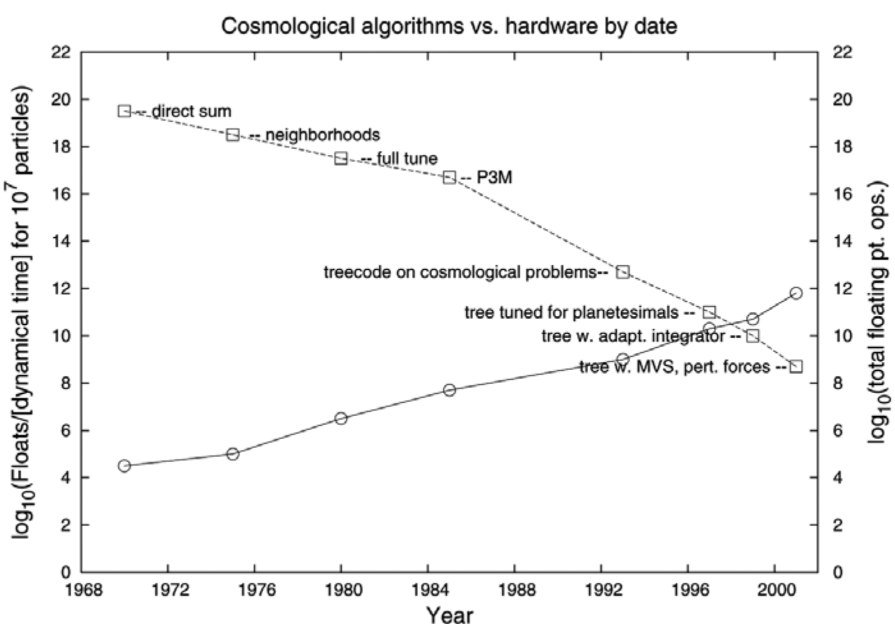

Figure 1. *Hardware advances versus improved algorithmic improvements. The hardware data are from a Linpack benchmark.*

In addition to smooth particle hydrodynamics schemes, large eddy simulation methods use particles supplemented by subgrid turbulence models. Shock-capturing upwind differencing coupled with conservation laws permits the study of hypersonic flows in colliding molecular clouds, x-ray emission in certain stars, and solar winds. Methods and approximations for modeling gravitational instabilities, magneto-hydro-dynamical couplings, and star formation began more than 40 years ago with Chandrasekar, Zel'dovich [11], and many others. The effects of turbulence are much more complicated, and improved numerical methods are needed. Turbulence effects are easily observed in star factories like the Orion and Eagle nebulae. Understanding such turbulence and its effects on energy dissipation and star formation is much harder. For example, models of *cold dense layers* in shock-bound regions require compressible hypersonic flow calculations [3]. Figure 3 illustrates model problems and computations for such systems.

Conclusions

Because astrophysical phenomena are almost entirely inaccessible to laboratory experiments, computer simulations are indispensable tools. Simulations are very complicated, however: Number scales span ten orders of magnitude, time scales fifteen orders of magnitude. In the 1960s, particle numbers in simulations were in the 100s. Today, systems with 10^9 massive particles are possible. Coupled with SPH or large eddy methods, gas dynamics, dark matter, and shock resolution can be examined to expand our theoretical understanding. Powerful computers are only part of the story. As shown in Figure 1, algorithm development has doubled the order of magnitude in resolution that hardware improvements have granted us.

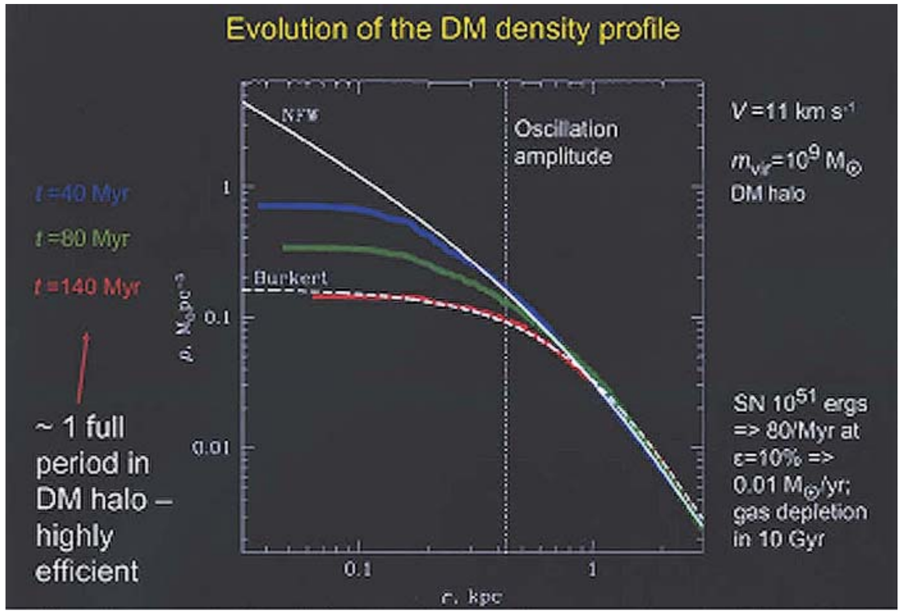

Figure 2. *Density profile vs. radius: flattening of cusps in galactic halos.*

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Wesley Petersen of ETH Zurich organized the two-part minisymposium Computational Methods in Astrophysics and Cosmology for ICIAM '07. George Lake, also of ETH Zurich, co-organized and spoke at the minisymposium. Hugh Couchman of McMaster University and Doris Folini of ETH Zurich gave talks during the sessions.

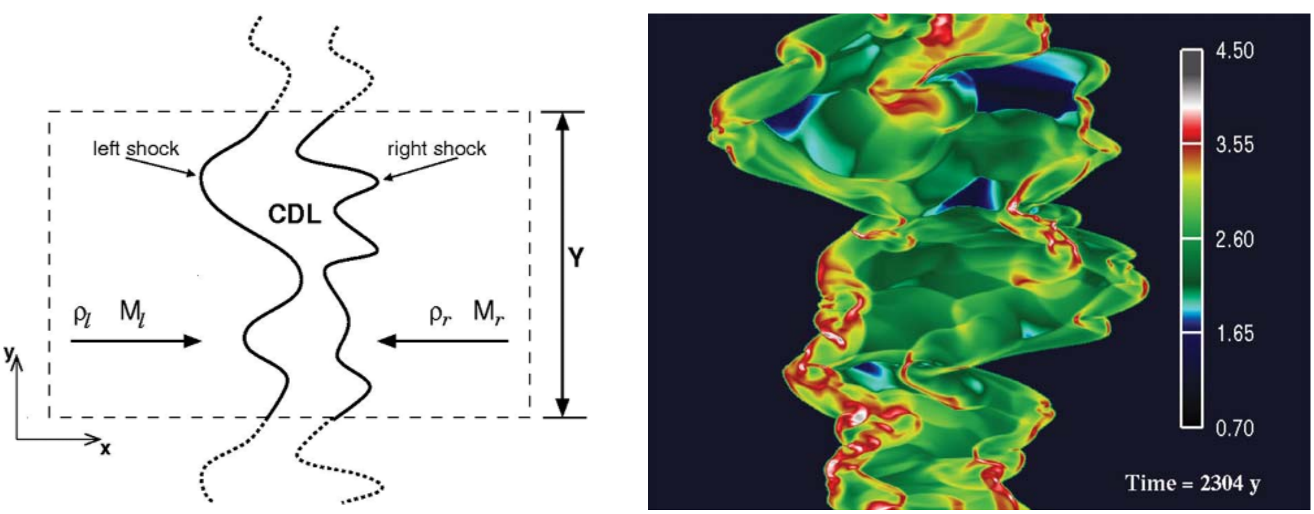

Figure 3. *Left, model setup for cold dense layer (CDL) simulations. The parameters ρ, M and s are the density and Mach number. Right, simulation of a CDL after long times. The color profile is the logarithm of the density.*